On the theory of Bose-condensate fluctuations in systems of finite size

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Abstract

An asymptotic expansion for the grand partition function of an ideal Bose gas is obtained for the canonical ensemble with arbitrary number of particles. It is shown that the expressions found are valid at all temperatures, including the critical region. A comparison of the asymptotic formulas for fluctuations of the Bose condensate with exact ones is carried out and their quantitative agreement is established. PACS: 05.30.Jp, 75.30.Ds, 75.70-i

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Introduction

The statistical mechanics of an ideal Bose gas [1, 2] is one of the simplest while at the same time fundamental subject areas of theoretical physics. The most impressive result of the theory is the remarkable phenomenon of Bose-Einstein condensation (BEC), which was in fact predicted by Einstein [3] the accumulation of an unlimited number of noninteracting (and this is also nontrivial) particles in their quantum ground state. We note that BEC turned out to be the first exactly solvable model of a phase transition and is a demonstration of the possibility of quantum behavior on macroscopic scales. Unfortunately, there are no substances in nature that satisfy the conditions of BEC in thermodynamic equilibrium. Nevertheless, the idea of the the Bose condensate has turned out to be very useful for understanding the essence of such remarkable physical phenomena as superfluidity and superconductivity and has been fruitful in various conceptual speculations in condensed matter physics and quantum field theory.

By the end of the last century experimental technique had been perfected so much that it became possible to restrain a cloud of polarized atoms of hydrogen or alkali metals in a magnetic trap long enough to cool it to very low temperatures ($\sim 20\, n\mathrm{K} \ldots \sim 1\, \mu\mathrm{K}$) [4,6–8] as a result, a large number of atoms ($\sim 10^3$ in the case of rubidium and $\sim 10^5$ for sodium) have been collected in the lowest-energy quantum state. Although it is understood

that it is not in a state of thermodynamic equilibrium, this is commonly regarded as the experimental preparation of a Bose condensate.

If one has in mind not a strict thermal equilibrium but a quasi-equilibrium, then it is entirely acceptable to consider a collective of some quasiparticles whose mutual interaction is also weak, as a rule, to be a suitable object for experimental investigation of BEC. As we know, the condition for thermal equilibrium here requires that the chemical potential vanish ($\mu = 0$), while the BEC regime corresponds to an increase of the chemical potential to the lowest energy level ($\mu \to \varepsilon_0$). In the case when ε_0 is small, an equilibrium gas of quasiparticles is found at the threshold of Bose condensation. However, in quasiequilibrium (e.g., under the influence of the external pump creating the quasiparticles) it is possible in principle to control the chemical potential, increasing it to values close to ε_0 and thereby satisfying the necessary conditions for BEC.

One can give examples of phenomena from everyday life in which the BEC of quasiparticles in essence takes place. For example, from the standpoint of the quantum theory of solids, such processes as the ringing of various vessels, the sounding of tuning forks, etc., that are just the BEC of phonons "pumped" by the striking impact or, in other words, the preparation of a phonon Bose condensate, which, in turn, generates coherent sound emission. Remarkably, all this occurs at normal temperatures and so does not require any special experimental contrivances. At the same time, serious efforts continue to be made in the investigation of the BEC of such quasiparticles as excitons and biexcitons in semiconductors [9] and magnons in certain classes of quantum magnets [10]. Perhaps the most impressive are the recent results of Demokritov and co-authors [11] with microfilms of yttrium iron garnet. Their Mandelstam-Brillouin scattering experiments cleared revealed a resonance peak in the spectral density of the distribution of magnons over states as a function of frequency in the vicinity of the minimum energy of the corresponding energy spectrum upon an increase of pumping below a certain threshold value. These experiments might be described as having created an analog of the "magnon tuning fork", and at high (room) temperatures.

Although it can be said that our present understanding of the various properties of Bose condensates of particles and quasiparticles is adequate, a number of unanswered questions remain, in particular, in regard to fluctuations of some observable quantities. This pertains primarily to systems of finite size or with a finite number of condensing particles, when the very concept of thermodynamic limit becomes problematical. Here it should be mentioned that the samples used in experiments on BEC are not only finite but usually small in size. If the spatial dimensions of the system are finite, then the statistical mechanics of the Bose gas is substantially complicated. In particular, the concept of equivalence of canonical ensembles loses meaning. We note here that in the BEC regime, inequivalence of ensembles is manifested even in the thermodynamic limit. Some finite-size effects for a Bose gas in a box were discussed in [12]. The "poor" behavior of fluctuations of the condensed particles described in the framework of the grand canonical ensemble (GCE) prompted the authors of [12] to draw the radical conclusion that this ensemble is unsuitable for describing any real physical system undergoing BEC. We add that the entropy also behaves "poorly" in the GCE - as the temperature goes to zero it does not go to zero in accordance with the Nernst theorem but, on the contrary, diverges (logarithmically) when the number of particles $N \to \infty$. However, the GCE, because of its simplicity, is extremely convenient for concrete calculations; moreover, the behavior of such quantities as, e.g., the number of particles in the ground state, N_0, or the specific

heat does not differ in calculations using different ensembles.

The experimental study of BEC in traps has revived the theoretical research on different aspects of the statistical mechanics of Bose systems [13]– [23]. This is primarily because of the fact that until then attention had mainly been devoted to a spatially homogeneous gas found in a certain volume. In the traps that were actually used the gas is inhomogeneous, and therefore the results obtained previously for a homogeneous Bose gas in a box can be reproduced for a trap by considering it to be a potential well with a harmonic law of spatial confinement, i.e., basically reducing the problem to a system of N oscillators.

Their partition function in the GCE (the grand partition function) is trivial to calculate. In the canonical (CE) and microcanonical (MCE) ensembles the corresponding partition functions are expressed in terms of contour integrals of the grand partition function. Therefore for not too large a number of particles and not very high energy, if one is talking about the MCE, the partition function of the Bose system can be calculated to any desired accuracy by the residue theorem or numerical integration. As to the analytical calculations of the partition function in the CE and MCE, one usually uses the saddle-point (steepest descent) method. However, as was shown in [12], for example, that method is inapplicable in the most interesting region - the neighborhood of the BEC, where the corrections to the main contribution do not fall off with increasing number of particles in the system.

A number of calculations have been done to investigate the thermodynamic properties of finite Bose systems in different statistical ensembles. In particular, in [13] the difference between the behavior of the number of condensate particles N_0 and also their fluctuations, calculated for a harmonic trap with the use of the GCE or CE when the total number of particles varied in the range $10^2 \leq N \leq 10^6$. In [14], which was devoted to a comparison of the results of an exact calculation in the MCE write approximate results obtained by the saddle-point method, it was noted that these results differ substantially precisely in the neighborhood of the BEC point.

Nevertheless, to this day there is no convenient analytical representation for the partition function in the CE and MCE which would correspond well enough to the BEC regime. The goal of the present study is to remedy this. In Sec. I we introduce the necessary notation and definitions and also obtain an analytical expression for the average number of particles N_0 on the ground level under the condition $N_0 \gg 1$. In the Sec. II we calculate the partition function in the CE by the saddle-point method with the first correction taken into account. In Sec. III we analyze why the domain of applicability of the saddle-point method is limited to temperatures $T > T_{BEC}$; here by isolating the singularity corresponding to the ground level, we derive an expression valid for $T < T_{BEC}$ as well. In Sec. IV we propose a method of asymptotic expansion of the partition function in the CE in inverse powers of the number of particles, which works both above and below the BEC temperature. On the basis of the representation obtained, we calculate the fluctuations of the Bose condensate and demonstrate the quantitative agreement with the exact result down to very small values of the number of particles in the system. In the Conclusion we discuss the BEC temperature for a harmonic trap and a box and also the difference of the mathematical mechanism of formation of the critical point in the GCE and CE.

1 Grand Canonical Ensemble

A stationary quantum system consisting of N noninteracting particles is known to be completely characterized by the configuration $[\mathrm{n}] = \{\mathrm{n}_0, \mathrm{n}_1, \mathrm{n}_2, \ldots\}$, where $\mathrm{n}_k = 0, 1, 2, \ldots$ is the number of particles in the kth quantum states $((k = 0, 1, 2, \ldots)$ According to the precepts of statistical mechanics, the (time) average of an observable quantity A in a nonstationary system coincides with to the average over an ensemble of stationary systems. An ensemble is determined by the distribution function $\rho[\mathrm{n}]$. Then

$$\overline{A} = Z^{-1} \sum_{[\mathrm{n}]} \rho[\mathrm{n}] A[\mathrm{n}] \,, \tag{1.1}$$

where the normalizing coefficient Z (the partition function) has the form

$$Z = \sum_{[\mathrm{n}]} \rho[\mathrm{n}] \,. \tag{1.2}$$

In the description of an ideal Bose gas one generally uses the GCE, with a distribution function

$$\rho[\mathrm{n}] = \mathrm{e}^{\sum\limits_k \mathrm{n}_k(\mu - \varepsilon_k)/T} \,, \tag{1.3}$$

where T is the temperature, μ is the chemical potential, and ε_k is the single-particle energy of the kth state. Here and below we have set Boltzmann's constant $k_B = 1$. Since $\rho[\mathrm{n}]$ (1.3) is factorized with respect to the dependence on the occupation numbers n_k, the summation over configurations $[\mathrm{n}]$ is trivial to do. In particular, the average number of particles in the kth state

$$\overline{\mathrm{n}}_k = Z^{-1} \sum_{[\mathrm{n}]} \rho[\mathrm{n}] \mathrm{n}_k = \frac{\sum\limits_{\mathrm{n}=0}^{\infty} \mathrm{n}\, \mathrm{e}^{\mathrm{n}(\mu - \varepsilon_k)/T}}{\sum\limits_{\mathrm{n}=0}^{\infty} \mathrm{e}^{\mathrm{n}(\mu - \varepsilon_k)/T}} = \frac{1}{\mathrm{e}^{(\varepsilon_k - \mu)/T} - 1} \,. \tag{1.4}$$

The function on the right-hand side of (1.4) specifies the average occupation number and, hence, is a constituent element of the expressions for the majority of thermodynamic quantities (and not only in the GCE), and it is deviate to use a special notation for it:

$$n_k = \frac{1}{\mathrm{e}^{(\varepsilon_k - \mu)/T} - 1} = \frac{1}{\mathrm{e}^{(\varepsilon_k - \varepsilon_0)/T}(1 + n_0^{-1}) - 1} \,. \tag{1.5}$$

With the use of (5) the partition function (1.2) is expressed as the product (1.5)

$$Z = \prod_{k=0}^{\infty} (n_k + 1) \,. \tag{1.6}$$

The independent variables in the GCE are assumed to be T and μ. However, as follows from Eq. (1.5), they could be considered to be the temperature and the number of particles n_0 in the (ground) state with the lowest energy ε_0, which facilitates the analysis of the different regimes of the GCE.

We write the average value of the total number of particles in the form

$$\overline{N} = \sum_{k=0}^{\infty} \overline{\mathrm{n}}_k = n_0 + N_{\mathrm{ex}}(n_0, T) \,, \tag{1.7}$$

where

$$N_{\text{ex}}(n_0,T) \equiv N_{\text{ex}} = \sum_{k=1}^{\infty} n_k \tag{1.8}$$

is the average number of particles in the excited states. If the value of $\overline{N}$ is fixed, then all the numbers n_k except n_0 fall with decreasing temperature ($n_{k\neq 0} = 0$ at $T = 0$), and n_0 grows to $n_0 = \overline{N}$ at $T = 0$. We denote by $\widetilde{n}_k$ the maximum possible value of the average occupation number at a given temperature, i.e., the value of n_k of Eq. (1.5) for $n_0 \to \infty$ (or, equivalently, $\mu = \varepsilon_0$):

$$\widetilde{n}_k = \frac{1}{\mathrm{e}^{(\varepsilon_k-\varepsilon_0)/T} - 1} \,. \tag{1.9}$$

Then for $n_0 \gg 1$ for the number n_k specified by Eq. (1.5) one can limit consideration to the expansion

$$n_k \simeq \widetilde{n}_k - \frac{\widetilde{n}_k(\widetilde{n}_k + 1)}{n_0} \,, \tag{1.10}$$

which, in turn, reduces Eq. (1.7) for n_0 to a simple quadratic equation:

$$\overline{N} = n_0 + \widetilde{N}_{\text{ex}} - \frac{\delta\widetilde{N}_{\text{ex}}^2}{n_0} \,, \tag{1.11}$$

in which

$$\widetilde{N}_{\text{ex}} = \sum_{k=1}^{\infty} \widetilde{n}_k \,, \qquad \delta\widetilde{N}_{\text{ex}}^2 = \sum_{k=1}^{\infty} \widetilde{n}_k(\widetilde{n}_k + 1) \tag{1.12}$$

is the maximum possible number of particles in excited states and its mean-square fluctuation. We note that the quantities marked with a tilde are functions of temperature only. The solution of equations (1.11) with respect to n_0 is denoted as

$$N_0(T) = \frac{1}{2}\left(\overline{N} - \widetilde{N}_{\text{ex}} + \sqrt{(\overline{N} - \widetilde{N}_{\text{ex}})^2 + 4\delta\widetilde{N}_{\text{ex}}^2}\right) , \tag{1.13}$$

which we shall call the Bose condensate. This terminology is conditional in the sense that one is considering a problem outside the thermodynamic limit, with a finite total number of particles $\overline{N}$. It follows from the definitions (1.9) and (1.12) that $\widetilde{N}_{\text{ex}}(T)$ and $\delta\widetilde{N}_{\text{ex}}^2(T)$ are monotonically increasing functions of temperature. We denote by T_c the temperature at which $\widetilde{N}_{\text{ex}}$ is equal to $\overline{N}$, which corresponds to

$$\widetilde{N}_{\text{ex}}(T_c) = \overline{N} \,. \tag{1.14}$$

If $\delta\widetilde{N}_{\text{ex}}^2 \ll (\overline{N} - \widetilde{N}_{\text{ex}})^2$, and this holds for $T \neq T_c$ and $\overline{N} \gg 1$, then the behavior of solution (1.13) in the limit $N \to \infty$ acquires a stepped character. For different temperature regions, both below T_c, where $\overline{N} > \widetilde{N}_{\text{ex}}$, and above T_c, where $\overline{N} < \widetilde{N}_{\text{ex}}$, the asymptotic behavior of $N_0(T)$ at large but finite $\overline{N}$ has the simple form

$$N_0(T) = \begin{cases} \overline{N} - \widetilde{N}_{\text{ex}}, & T < T_c, \\ \delta\widetilde{N}_{\text{ex}}, & T = T_c, \\ \delta\widetilde{N}_{\text{ex}}^2/(\widetilde{N}_{\text{ex}} - \overline{N}), & T > T_c \end{cases} . \tag{1.15}$$

The value of T_c at which the change of regime (the crossover) in the behavior of $N_0(T)$ occurs can be regarded as a generalization of the temperature $T_{\rm BEC}$ to the case of a finite number of particles in the system. We recall that Eq. (1.11) is approximate, in accordance with the condition $n_0 \gg 1$. In the opposite case, when $n_0 \ll 1$ (the Boltzmann limit), Eq. (1.7) gives the simple depends

$$N_0(T) \simeq \frac{\overline{N}}{1+Q(T)}\,, \qquad Q(T) = \sum_{k=1}^{\infty} \mathrm{e}^{-(\varepsilon_k-\varepsilon_0)/T}\,, \tag{1.16}$$

which attest to the classical behavior of the Bose systems under consideration.

Independently of the number of particles n_0 in the condensate the factorized character of the distribution function (1.3) in the GCE is conditional upon the absence of any correlations between particles of the Bose gas in different quantum states. This has the consequence

$$\overline{\mathrm{n}_k\mathrm{n}_l} = \overline{\mathrm{n}}_k \cdot \overline{\mathrm{n}}_l\,. \tag{1.17}$$

The average of the square (and higher powers) of the number of particles in the kth state is calculated in analogy with Eq. (1.4):

$$\overline{\mathrm{n}_k^2} = 2n_k^2 + n_k\,, \tag{1.18}$$

from which the mean-square deviation (or, in other words, the mean-square fluctuation) is easily calculated and has the form

$$\delta\mathrm{n}_k^2 = \overline{\mathrm{n}_k^2} - \overline{\mathrm{n}}_k^{\,2} = n_k(n_k+1). \tag{1.19}$$

Taking Eq. (1.17) into account, we write the square of the fluctuation of the total number of particles as

$$\delta N^2 = \delta\mathrm{n}_0^2 + \delta N_{\rm ex}^2, \quad \delta\mathrm{n}_0^2 = n_0(n_0+1), \quad \delta N_{\rm ex}^2 = \sum_{k=1}^{\infty} n_k(n_k+1). \tag{1.20}$$

For $T < T_c$ the value $\mathrm{n}_0 \sim \overline{N}$, and the square of the fluctuation of the number of condensed particles is

$$\delta\mathrm{n}_0^2 = n_0(n_0+1) \sim \overline{N}^{\,2}. \tag{1.21}$$

Thus the relative fluctuation $(\delta\mathrm{n}_0^2/\overline{N})^{1/2}$ grows with increasing number of particles in the system, and this is the basis for the widespread assertion that the fluctuations diverge below the BEC point (see, e.g., [2]).

We note in this regard that the description of the BEC in the framework of the GCE cannot be considered quite correct, if for no other reason that it explicitly violates the Nernst theorem. Indeed, the entropy of the GCE is expressed in terms of the average occupation number as

$$S = \sum_k [(n_k+1)\ln(n_k+1) - n_k \ln n_k]. \tag{1.22}$$

In the region $T \ll T_c$, where $n_0 \gg 1$ and $n_{k\neq 0} \ll 1$, it becomes equal to the entropy of the Bose condensate:

$$S \simeq (n_0+1)\ln(n_0+1) - n_0\ln n_0 \simeq \ln(n_0+1) + 1.$$

When $T \to 0$, the entropy $S \simeq \ln \overline{N}$, i.e., not only does it not go to zero but it diverges with increasing number $\overline{N}$. As will be seen below, in the canonical ensemble there is no problem with a divergence of the fluctuations nor with the entropy.

2 Canonical Ensemble

The main difference between the CE and GCE is that the total number of particles in the CE is rigidly fixed: $N = \sum\limits_{k=0}^{\infty} \mathrm{n}_k = \mathrm{n}_0 + N_{\mathrm{ex}}$. From this it follows directly that

$$\overline{\mathrm{n}}_0 = N - \overline{N}_{\mathrm{ex}}, \tag{2.1}$$

$$\overline{(\mathrm{n}_0 - \overline{\mathrm{n}}_0)^2} = \overline{(N_{\mathrm{ex}} - \overline{N}_{\mathrm{ex}})^2}, \tag{2.2}$$

i.e., the fluctuation of the Bose condensate does not differ from the fluctuation of the total number of particles in excited states, or

$$\delta \mathrm{n}_0 = \delta N_{\mathrm{ex}}. \tag{2.3}$$

It is essential here that in the CE the average number of particles in the k th state is not equal to the average occupation number, determined in Eq. (1.5), and the noninteracting particles in different quantum states (in contrast to the GCE) are correlated with each other.

The fluctuation of the Bose condensate in the CE can be estimated starting from the following qualitative arguments. For $T > T_c$ the number $\overline{\mathrm{n}}_0 \ll N$. Therefore, considering the Bose condensate as a small subsystem, one can suppose that a description of it in the framework of the GCE is valid. Consequently, for $T > T_c$ the following relation also holds in the CE [see Eq. (1.19)]:

$$\delta \mathrm{n}_0^2 \simeq n_0(n_0 + 1). \tag{2.4}$$

When $T < T_c$, however, the small subsystem becomes the particles above the condensate, and now the mean-square fluctuation of their number in the CE can be described by the expression

$$\delta N_{\mathrm{ex}}^2 \simeq \sum_{k=1}^{\infty} n_k(n_k + 1). \tag{2.5}$$

Doing a simple interpolation of expressions (2.4) and (2.5) with (2.3) taken into account, we find that

$$\delta \mathrm{n}_0^2 = \delta N_{\mathrm{ex}}^2 = \frac{n_0(n_0+1) \sum\limits_{k=1}^{\infty} n_k(n_k+1)}{\sum\limits_{k=0}^{\infty} n_k(n_k+1)}. \tag{2.6}$$

Below we compare this phenomenological expression with the expression calculated directly in the CE.

For this we define the distribution function in the CE [cf. Eq. (1.3)]

$$\rho[\mathrm{n}] = \mathrm{e}^{-\sum\limits_k \mathrm{n}_k \varepsilon_k / T} \delta(N - \sum_k \mathrm{n}_k). \tag{2.7}$$

The property of factorization of $\rho[\mathrm{n}]$ is lost because of the presence of the δ-function on the right-hand side of Eq. (2.7), so that in comparison with the GCE the calculation of the partition function and the averages of the observables is complicated. Factorizability can be easily restored, however, and the summation over configurations $[\mathrm{n}]$ can be reduced to

a summation over independent n_k if one uses the integral representation of the Kronecker δ-function:

$$\delta(m) = \frac{1}{2\pi}\int\limits_{-\pi}^{\pi} dx\, \mathrm{e}^{ixm}. \tag{2.8}$$

Then, substituting (2.8) into (2.7) and changing the sequence of summation and integration, we arrive at the following representation for the partition function:

$$Z = \frac{1}{2\pi}\int\limits_{-\pi}^{\pi} dx\, \mathrm{e}^{ixN} \sum_{[\mathrm{n}]} \mathrm{e}^{-\sum\limits_k \mathrm{n}_k(\varepsilon_k/T+ix)} = \frac{1}{2\pi}\int\limits_{-\pi}^{\pi} dx\, \mathrm{e}^{ixN+W(-ix)}\,, \tag{2.9}$$

where

$$W(-ix) = -\sum_k \ln(1-\mathrm{e}^{-\varepsilon_k/T-ix}),$$

or, denoting x as $i\nu$,

$$W(\nu) = \sum_{k=0}^{\infty} \ln(n_k+1), \qquad n_k = \frac{1}{\mathrm{e}^{\varepsilon_k/T-\nu}-1}\,. \tag{2.10}$$

A comparison of Eqs. (2.10) and (1.6) shows that the function $W(\nu)$ is the logarithm of the partition function in the GCE if one sets $\nu = \mu/T$. Thus in the CE the averages of physical quantities are just the ratios of the corresponding integrals of the same averages found in the GCE. This, on the one hand, establishes a definite relation between the two statistical ensembles and, on the other, allows one to use the initial [see Eq. (1.5)] definition for the number of Bose particles in each of the states. However, in them the average in the CE can also be expressed in terms of derivatives of the partition function. For example, in the simplest case of a nondegenerate spectrum ε_k we have

$$\overline{\mathrm{n}}_k = Z^{-1}\sum_{[\mathrm{n}]}\rho[\mathrm{n}]\mathrm{n}_k = -Z^{-1}T\frac{\partial}{\partial\varepsilon_k}\sum_{[\mathrm{n}]}\rho[\mathrm{n}] = -T\frac{\partial \ln Z}{\partial \varepsilon_k}\,, \tag{2.11}$$

$$\delta\mathrm{n}_k^2 = -T\frac{\partial\overline{\mathrm{n}}_k}{\partial\varepsilon_k}\,. \tag{2.12}$$

At large N the integral on the right-hand side of Eq. (2.9) can be evaluated by the saddle-point method, which leads to the following asymptotic expansion:

$$Z = \frac{\mathrm{e}^{W(\nu)-\nu N}}{\sqrt{2\pi W''(\nu)}}(1+z_1+z_2+\cdots). \tag{2.13}$$

Here ν denotes the saddle point nearest to the origin of coordinates in the complex x-plane $(x_s = i\nu)$, the equation for which has the form

$$W'(\nu) = \sum_{k=0}^{\infty} n_k = N. \tag{2.14}$$

In the leading asymptotic approximation the logarithm of the partition function in the CE has the following simple form:

$$\ln Z = W(\nu) - \nu N - \tfrac{1}{2}\ln[2\pi W''(\nu)]. \tag{2.15}$$

The contributions z_j in Eq. (2.13) are expressed in terms of ratios of the derivatives of the function $W(\nu)$ of the type

$$\frac{[W^{(l)}(\nu)]^m [W^{(k)}(\nu)]^n}{[W''(\nu)]^{m+n+j}} . \tag{2.16}$$

If the function $W(\nu)$ and its derivatives are large, $W^{(l)}(\nu) \sim N$, and this is the case at least in the region $T > T_c$ and $N \gg 1$, then the ratios (2.16) and the contributions z_j have order of smallness $O(N^{-j})$. Thus for the first correction we find:

$$z_1 = \frac{W^{(4)}(\nu)}{8[W''(\nu)]^2} - \frac{5[W'''(\nu)]^2}{24[W''(\nu)]^3} = O(N^{-1}). \tag{2.17}$$

We take the derivative of the occupation number (2.10) with respect to ε_l:

$$T\frac{\partial n_k}{\partial \varepsilon_l} = n_k(n_k+1)\left(T\frac{\partial \nu}{\partial \varepsilon_l} - \delta_{kl}\right). \tag{2.18}$$

The derivative of the saddle point ν with respect to ε_l is evaluated by differentiating Eq. (2.14):

$$T\frac{\partial \nu}{\partial \varepsilon_l} = \frac{n_l(n_l+1)}{W''(\nu)} . \tag{2.19}$$

Now with the aid of Eqs. (2.11), (2.15), (2.18), and (2.19) we find the average value of the number of particles in the kth state,

$$\overline{\mathrm{n}}_k = n_k - \frac{n_k(n_k+1)}{2W''(\nu)}\left(2n_k + 1 - \frac{W'''(\nu)}{W''(\nu)}\right) . \tag{2.20}$$

In particular, for the average number of particles in the ground state (2.11) we obtain

$$\overline{\mathrm{n}}_0 = n_0 - \frac{n_0(n_0+1)}{2W''(\nu)^2}\left[(2n_0+1)V''(\nu) - V'''(\nu)\right], \tag{2.21}$$

where $V(\nu)$ denotes the sum over only the excited states,

$$V(\nu) = W(\nu) - \ln(n_0+1) = \sum_{k=1}^{\infty} \ln(n_k+1). \tag{2.22}$$

finally, differentiating $\overline{\mathrm{n}}_0$ with respect to ε_0 [see Eq. (2.12)], we arrive at an expression for the mean-square fluctuation of the Bose condensate:

$$\delta \mathrm{n}_0^2 = \delta_1 + \delta_2 + \delta_3 , \tag{2.23}$$

with the leading contributions

$$\delta_1 = \frac{n_0(n_0+1)V''(\nu)}{W''(\nu)} , \tag{2.24}$$

$$\begin{aligned}\delta_2 = {} & \frac{\delta_1}{2W''(\nu)^2}\Bigg\{(2n_0+1)V'''(\nu) - (6n_0^2+6n_0+1)V''(\nu) + \\ & + \frac{2n_0(n_0+1)(2n_0+1)}{W''(\nu)}\left[(2n_0+1)V''(\nu) - V''(\nu)\right]\Bigg\} ,\end{aligned} \tag{2.25}$$

$$\begin{aligned}\delta_3 = {} & \frac{n_0^2(n_0+1)^2}{2W''(\nu)^3}\Bigg\{(2n_0+1)V'''(\nu) - V^{(4)}(\nu) - \\ & - \frac{2V'''(\nu)}{W''(\nu)}\left[(2n_0+1)V''(\nu) - V'''(\nu)\right]\Bigg\} .\end{aligned} \tag{2.26}$$

In the temperature region $T > T_c$ the condensate is dilute, $n_0 \ll N$, and, accordingly,

$$\delta_1 \simeq n_0(n_0+1), \quad \delta_2 \sim \frac{\delta_1}{N}, \quad \delta_3 \sim \frac{\delta_1^2}{N^2}. \tag{2.27}$$

We note that the phenomenological formula (2.6) for the fluctuation of the Bose condensate coincides with the leading asymptotic contribution δ_1 (2.24).

An exact expression for the partition function is given by the single integral (2.9), which for not too large N is easily found numerically. It is interesting here to compare the exact expression for the fluctuations with its asymptotic behavior given by formulas (2.23)–(2.26). Such a comparison, however, is impossible to do in general form, since the quantitative calculations require specifying the explicit form of the function $W(\nu)$, which, in turn, depends on the concrete form of the energy spectrum ε_k. Let us find it for the case of alkali metal atoms in magnetic traps.

Experiments on cooling of a large number of alkali metal atoms $(N \simeq 10^3 \ldots 10^4)$ are interpreted as the experimental realization of BEC. The particles are confined in the traps by a potential $v(\mathbf{r})$, the exact dependence of which on the distance $\mathbf{r}$ is, gives speaking, unknown, but for theoretical analysis usually a quadratic (harmonic) approximation is used. As a result, the problem of BEC reduces, as we have said, to a calculation of the partition function of a system of linear oscillators. The spectrum ε_l and the spectral density g_l (coefficient of degeneracy) of the three-dimensional isotropic oscillator has the simple form

$$\begin{aligned} &\varepsilon_l = \hbar\omega\big(l + \tfrac{3}{2}\big), \quad g_l = \tfrac{1}{2}(l+1)(l+2), \quad l = 0, 1, 2, \ldots\,, \\ &g(\varepsilon) = \frac{1}{2}\left(\frac{\varepsilon^2}{\hbar^2\omega^2} - \frac{1}{4}\right), \quad \varepsilon_0 = \frac{3}{2}\hbar\omega. \end{aligned} \tag{2.28}$$

We point out that in Eq. (2.28) the index l enumerates the energy levels and not quantum states, which are enumerated by the index k introduced previously. At high temperatures $(T \gg \varepsilon_0)$ the series expressions for the function $W(\nu)$ and its derivatives converge slowly. It is shown in the Appendix how to improve their convergence and to obtain expressions convenient for numerical calculations.

The equation for the crossover point in the CE differs from the equation (1.14) in the GCE by only the replacement of $\overline{N}$ by N, i.e.,

$$\widetilde{N}_{\text{ex}}(T_c) = N. \tag{2.29}$$

It follows from definitions (1.12) and (2.14) that $\widetilde{N}_{\text{ex}} = W'(\frac{\varepsilon_0}{T}) - \widetilde{n}_0$. Then, using for $W'(\nu)$ the asymptotic expansion [Eq. (A.21) in the Appendix] for high temperatures $\tau = T/\hbar\omega \gg 1$, we write the following expansion for $\widetilde{N}_{\text{ex}}$:

$$\widetilde{N}_{\text{ex}} = \tau^3\zeta(3) + \frac{3}{2}\tau^2\zeta(2) + \tau\ln\tau + O(\tau), \tag{2.30}$$

where $\zeta(j)$ is the Riemann ζ-function. From it we can find the solution of equation (2.29) that determines the crossover point τ_c in the form of an expansion in inverse powers of N. In the leading approximation we denote this solution as

$$\tau_{\text{BEC}} \equiv \frac{T_{\text{BEC}}}{\hbar\omega} = \left[\frac{N}{\zeta(3)}\right]^{1/3}. \tag{2.31}$$

Now, knowing equation (2.31), we find for τ_c from (2.29) and (2.30)

$$\frac{\tau_c}{\tau_{\rm BEC}} = \frac{T_c}{T_{\rm BEC}} = 1 - \frac{1}{\zeta(3)\tau_{\rm BEC}}\left[\frac{\zeta(2)}{2} + \frac{\ln \tau_{\rm BEC}}{3\tau_{\rm BEC}}\right] + O(\tau_{\rm BEC}^{-2}). \tag{2.32}$$

It is seen from expressions (2.31) and (2.32) that the crossover temperature T_c is below the condensation temperature $T_{\rm BEC}$ for a Bose gas in a trap. We note that for a Bose gas in a box the situation is the opposite, $T_c > T_{\rm BEC}$.

Expressions (2.31) and (2.32) with the known numerical values of the ζ-function in them easily convince one that even for a number of particles of the order of 10^3 the condensation temperature T_c is only 6 times greater than the ground-state energy ε_0. This is a direct indication that the condensation phenomenon observed in the experiments mentioned is of a microscopic (or, in any case, mesoscopic) rather than macroscopic character. This casts doubt on whether the condensation of several thousand particles can be regarded unambiguously as BEC, the main feature of which, strictly speaking, is the appearance and manifestation of quantum properties in macroscopic phenomena or objects.

Without denying, of course, the presence of the phenomenon of BEC itself in magnetic traps, we would nevertheless like to say that, in our view, the results set forth in this Section are evidence that the condensation of alkali metal atoms observed in the experiments is more of a nanophysical character.

In Fig. 1 we show graphs of the fluctuations of the Bose condensate in the case of their exact calculation,

$$\delta {\rm n}_0^2 = T^2\,\frac{\partial^2 \ln Z}{\partial \varepsilon_0^2}$$

and their approximate calculation (2.23)–(2.26). It is seen that the asymptotic expressions represented by Eq. (2.23) and the corrections to it do not adequately reproduce the curve of the numerical calculation.

3 Bose-Einstein Condensation Region $T < T_c$

Let us consider in more detail the low-temperature region, where one can more or less definitely talk about the presence of a Bose condensate. As we have said (see Fig. 1), here the discrepancy between the exact and asymptotic values of the fluctuations are significant. The reason is not hard to understand. The fact is that in the region $T < T_c$ the evaluation of integral (2.9) by the straightforward saddle-point method does not actually give the asymptotic expansion in inverse powers of N: the terms z_1, $z_2, \ldots$ in Eq. (2.13) do not fall with increasing N. The contributions of the ground term w_0 to the sum $W(\nu) = \sum\limits_{k=0}^{\infty} w_k$ (2.10) and its derivatives with respect to ν are:

$$w_0 = \ln(n_0+1), \quad w_0' = n_0, \quad w_0'' = n_0(n_0+1), \quad w_0''' = n_0(n_0+1)(2n_0+1).$$

Since for $T < T_c$ the pth order derivative $w_0^{(p)} \sim n_0^p \sim N^p$, for the first correction, e.g., we have

$$z_1 \simeq \frac{1}{8}\frac{n_0(n_0+1)(6n_0^2+6n_0+1)}{n_0^2(n_0+1)^2} - \frac{5}{24}\frac{n_0^2(n_0+1)^2(2n_0+1)^2}{n_0^3(n_0+1)^3} \simeq -\frac{1}{12}\,.$$

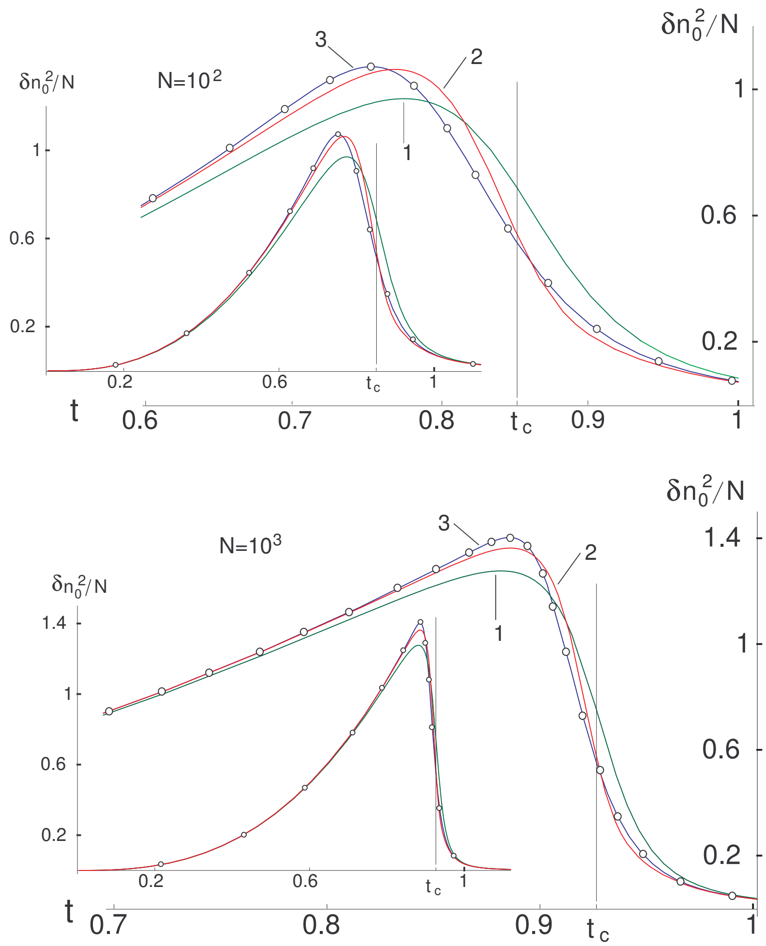

Рис. 1: The dependence on temperature $t = T/T_{BEC}$ of the relative fluctuation of the Bose condensate $\delta n_0^2/N$. The circlets denote the results of a numerical calculation of the integral in Eq. (2.9). Curve 1 is the leading contribution to the asymptotic expansion (2.23), curve 2 is with the next correction to Eq. (2.23) taken into account, and curve 3 is the asymptotic expansion (4.11), (4.14).

It is not hard to show that the other contributions z_j in (2.13) not only do not fall with increasing N but even grow with increasing j. Nevertheless, the problem of singular behavior of the contributions corresponding to the ground state can be solved as follows.

We denote by $U(-ix)$ the exponent of the integrand in Eq. (2.9):

$$U(-ix) = ixN + W(-ix). \tag{3.1}$$

It follows from the definition of $W(\nu)$ [see Eq. (2.10)] that the function $U(-ix)$ is singular at the points $x_l = i\varepsilon_l/T$, and its real part goes to infinity at these points. Of course, the function $U(-ix)$ reaches its minimum value at points $i\nu_l$ lying along the imaginary axis between each pair of singular points:

$$U'(\nu_l) = 0, \quad \frac{\varepsilon_{l-1}}{T} < \nu_l < \frac{\varepsilon_l}{T}.$$

The behavior of the function $U(\nu)$ in the vicinity of the first singularity x_0 is shown schematically in Fig. 2.

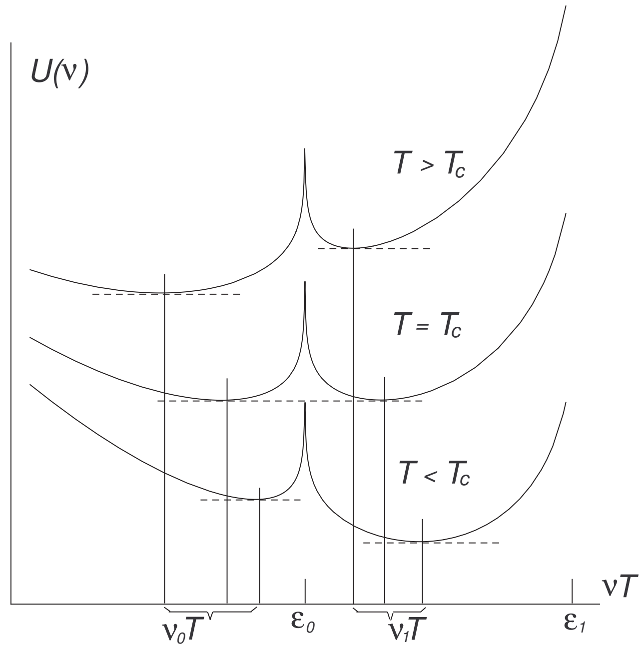

Рис. 2: Behavior of the function $U(\nu)$ in the vicinity of $\nu = \varepsilon_0/T$.

The depth of the minimum of the function $U(\nu)$ at the saddle points ν_0 and ν_1 depends on temperature: $U(\nu_0) < U(\nu_1)$ for $T > T_c$ and, oppositely, $U(\nu_0) > U(\nu_1)$ for $T < T_c$. Therefore for an optimal estimate of the integral (2.9) for $T < T_c$ the integration contour must be deformed so that it passes through the saddle point $x_s = i\nu_1$, as shown in Fig. 3. At the point x_0 the function $\exp[U(-ix)]$ has a simple pole. The contribution from this pole to the integral (2.9), which we denote Z_0 , is equal to the residue of the integrand there:

$$\ln Z_0 = -\frac{N\varepsilon_0}{T} + V\left(\frac{\varepsilon_0}{T}\right), \tag{3.2}$$

where the divergence $V(\nu)$ is defined in Eq. (2.22). The contribution of the integral along the contour C has the form

$$Z_1 = \frac{1}{2\pi}\int\limits_C dx\, \mathrm{e}^{U(-ix)} \simeq \frac{\mathrm{e}^{U(\nu_1)}}{\sqrt{2\pi U''(\nu_1)}}\,. \tag{3.3}$$

We note that, as a consequence of the periodicity of the function $W(\nu)$, i.e.,

$$W(\nu + 2\pi i) = W(\nu),$$

the contributions from the parts of the integration contour along the ray $[-\pi,\, -\pi + i\infty)$ and $[\pi,\, \pi + i\infty)$, being equal in magnitude and opposite in sign, cancel each other out. Furthermore, it is easy to see from expressions (3.2) and (3.3) that for $T < T_c$ and $N \gg 1$ the ratio of the integrals Z_1/Z_0 is exponentially small, and therefore the partition function in the BEC regime is given by the exceedingly simple expression (3.2). It follows from that expression, in particular, that the entropy

$$S = \frac{\partial \ln(T \ln Z_0)}{\partial T} = \sum_{k=1}^{\infty} [\ln(\widetilde{n}_k + 1) + \widetilde{n}_k(\varepsilon_k - \varepsilon_0)/T]\,,$$

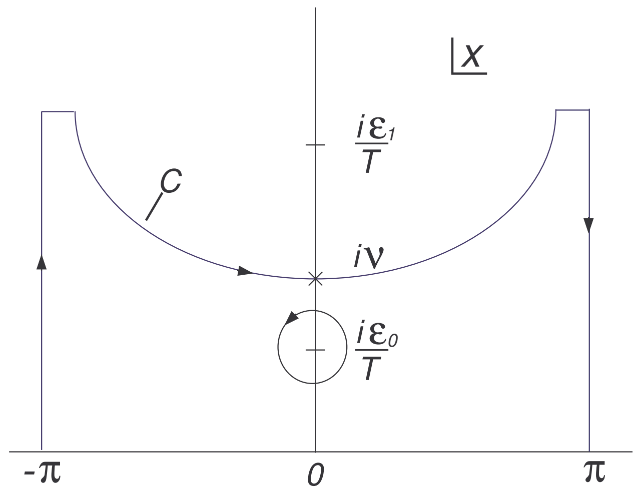

Рис. 3: Integration contour for the integral in Eq. (2.9) for $T < T_c$.

goes to zero at $T \to 0$, as it should.

4 Modified Asymptotic Expansion of the Partition Function

The most interesting region, but the hardest for calculations, is the critical neighborhood of T_c. Here the contributions of Z_0 and Z_1 are of the same order of magnitude, and the fluctuations are maximal. To obtain the correct asymptotic expansion of the integral (2.9) in inverse powers of the number of particles N we propose the following approach, consisting of several steps.

i) In the first step we separate out explicitly the first singular term in the integrand of (2.9):

$$Z = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dx \; \mathrm{e}^{U(-ix)}}{2\,\mathrm{sh}\left(\frac{\varepsilon_0}{2T} + \frac{ix}{2}\right)}\,, \tag{4.1}$$

where, in contrast to (3.1), the function U(-ix) here has a different form:

$$U(-ix) = \frac{\varepsilon_0}{2T} + ix(N + \tfrac{1}{2}) + V(-ix). \tag{4.2}$$

The saddle point $x_s = i\nu$ for the function (4.2) satisfies the equation [cf. Eq. (2.14)]

$$V'(\nu) = N + \tfrac{1}{2}. \tag{4.3}$$

ii) In the second step we make the change of integration variable $x \to u$:

$$u^2 = U(\nu) - U(-ix) = V(\nu) - V(-ix) - (\nu + ix)(N + \tfrac{1}{2}), \tag{4.4}$$

$$2u\,du = iU'(-ix) = i[V'(-ix) - N - \tfrac{1}{2}]. \tag{4.5}$$

iii) Finally, we deform the integration contour in the x-plane so that it passes through the saddle point along the line of steepest descent, which is determined by the equation

$$\mathrm{Im}[U(-ix)] = 0.$$

As a result of these steps we can transform the integral in (4.1) to a form in which

$$Z = Z_0 + Z_1, \tag{4.6}$$

$$Z_0 = \frac{\mathrm{e}^{U(\nu)}}{2\pi} \int_{-\infty}^{\infty} \frac{du\ \mathrm{e}^{-u^2}}{v + iu}, \tag{4.7}$$

$$Z_1 = \frac{\mathrm{e}^{U(\nu)}}{2\pi} \int_{-\infty}^{\infty} du\ \mathrm{e}^{-u^2} f(u), \tag{4.8}$$

and denote by iv the value of the variable u, defined in Eq. (4.4), corresponding to the point $x = i\varepsilon_0/T$:

$$v^2 = U(\tfrac{\varepsilon_0}{T}) - U(\nu) = V(\tfrac{\varepsilon_0}{T}) - V(\nu) - (\tfrac{\varepsilon_0}{T} - \nu)(N + \tfrac{1}{2}). \tag{4.9}$$

The function $f(u)$ in the integrand of (4.8) is analytic in the neighborhood of the point $u = iv$:

$$f(u) = \frac{u}{iU'[-x(u)]} \frac{1}{\mathrm{sh}[\frac{\varepsilon_0}{2T} + \frac{ix(u)}{2}]} - \frac{1}{v + iu}, \tag{4.10}$$

where the function $x(u)$ in (4.10) is determined by Eq. (4.4). The integral in (4.7) can be expressed in terms of the error function:

$$Z_0 = \tfrac{1}{2}\,\mathrm{e}^{U(\nu)+v^2} \mathrm{Erfc}\,(v) = \tfrac{1}{2}\,\mathrm{e}^{V(\varepsilon_0/T) - N\varepsilon_0/T} \mathrm{Erfc}\,(v), \tag{4.11}$$

which satisfies the well-known equations [24]

$$\mathrm{Erfc}\,(v) = \frac{2}{\sqrt{\pi}} \int_{v}^{\infty} dx\ \mathrm{e}^{-x^2}, \quad \mathrm{Erfc}\,(0) = 1, \quad \mathrm{Erfc}\,(-\infty) = 2, \quad \mathrm{Erfc}\,(-v) = 2 - \mathrm{Erfc}\,(v), \tag{4.12}$$

and, for $v \gg 1$, it has the asymptotic expansion

$$\mathrm{Erfc}\,(v) = \frac{\mathrm{e}^{-v^2}}{v\sqrt{\pi}} \left(1 - \frac{1}{2v^2} + \frac{3}{4v^4} + O(v^{-6})\right). \tag{4.13}$$

We find an approximate value of the integral (4.8) by expanding the function (4.10) in a Taylor series at the point $u = 0$:

$$Z_1 = \frac{\mathrm{e}^{U(\nu)}}{2\sqrt{\pi}} [f(0) + \tfrac{1}{4} f''(0) + \cdots]. \tag{4.14}$$

It follows from Eq. (4.5) that $dx/du = -2iu/U'(ix)$. Ultimately we obtain for the function $f(u)$ and its second derivative at the point $u = 0$

$$\begin{aligned} f(0) &= \frac{1}{\sqrt{2V''(\nu)}\,\mathrm{sh}(\frac{\varepsilon_0}{2T} - \frac{\nu}{2})} - \frac{1}{v}, \\ f''(0) &= \frac{2}{v^3} - \frac{2}{[2V''(\nu)]^{3/2}\,\mathrm{sh}(\frac{\varepsilon_0}{2T} - \frac{\nu}{2})} \times \\ &\times \left[\frac{1}{\mathrm{sh}^2(\frac{\varepsilon_0}{2T} - \frac{\nu}{2})} - \frac{V'''(\nu)}{V''(\nu)} \coth(\frac{\varepsilon_0}{2T} - \frac{\nu}{2}) + \frac{5}{6}\left(\frac{V'''(\nu)}{V''(\nu)}\right)^2 - \frac{V^{(4)}(\nu)}{2V''(\nu)} + \frac{1}{2}\right]. \end{aligned} \tag{4.15}$$

In the limit $T \to T_c$ we have $\nu \to \varepsilon_0/T$, $v \to 0$. Then, resolving the uncertainty $(\infty - \infty)$ at the point $v = 0$, we obtain from (4.15) for the crossover region

$$
\begin{aligned}
f(0) &= \frac{V^{(''')}(\nu)}{3\sqrt{2}[V''(\nu)]^{3/2}}, \\
f''(0) &= \frac{V'''(\nu)}{3\sqrt{2}[V''(\nu)]^{5/2}}\left[1 - \frac{35}{9}\left(\frac{V'''(\nu)}{V''(\nu)}\right)^2 + \frac{5V'''(\nu)}{V''(\nu)} - \frac{6V^{(5)}(\nu)}{5V'''(\nu)}\right].
\end{aligned}
\tag{4.16}
$$

The contributions $f(0)$, $f''(0)$, and their ratio $f''(0)/f(0)$ all fall off with increasing N. The power of the decrease of the ratio $f''(0)/f(0)$ depends on the asymptotic behavior of the derivatives $V^{(p)}(\nu)$, which, in turn, is determined by the concrete form of the spectrum ε_l or the spectral density g_l as functions of l. For the quadratic confining potential considered in the Appendix, the derivatives $V^{(p)} \sim N$ for $p < 3$, $V^{(3)} \sim N \ln N$ and $V^{(p)} \sim N^{p/3}$ for $p > 3$. It follows from this that representations (4.11) and (4.14) for the contributions to the partition function are indeed asymptotic expansions in inverse powers of N for all temperatures, including the critical temperature region $T \sim T_c$.

As we see from Figs. 2 and 4, even at relatively small numbers of particles (as low as $N \sim 100$) the discrepancy between the exact expressions for the fluctuations of the Bose condensate and the approximate expressions corresponding to the representation of the partition function in Eqs. (4.6), (4.11), (4.14), and (4.15) is indiscernable on the graphs. It can be shown that at a temperature below T_c the given representation coincides with the asymptotic expression (3.2), and for $T > T_c$ it goes over to (2.13).

The critical region is determined by the condition

$$
|\mathrm{Erfc}\,(v) - 1| \leqslant \epsilon, \quad \epsilon \ll 1. \tag{4.17}
$$

For example, setting $\epsilon = 10^{-1}$, we find from (4.17) the boundary value $v_\epsilon = 1.16$ and, using the asymptotic approximation for $V(\nu)$ [see Eq. (A.21) in the Appendix], we obtain for the critical temperature region $|T - T_c| \leqslant \Delta T$

$$
\frac{\Delta T}{T_{\mathrm{BEC}}} = \frac{\Delta\tau}{\Delta\tau_{\mathrm{BEC}}} = v_\epsilon\left(\frac{2}{\zeta(2)}\right)^{1/2}\left(\frac{\zeta(3)}{N}\right)^{1/3} \simeq \frac{1}{N^{1/3}}. \tag{4.18}
$$

It is seen from Eq. (4.18) that this region narrows extremely slowly with increasing particle number. In other words, the thermodynamic limit is reached at very large particle numbers $N \gtrsim 10^6$. Figure 5 illustrates the evolution of the relative fluctuation of the density of the Bose condensate as the total number of particles in the system is varied. The curves shown convincingly demonstrate that even for a system with $N \approx 10^4$ the temperature behavior of these fluctuations nevertheless differs markedly from the limit $N \to \infty$, in which

$$
\frac{\delta \mathrm{n}_0^2}{N} = \frac{V''(\varepsilon_0/T)}{N}\,\theta(T_{\mathrm{BEC}} - T) = \frac{\zeta(2)}{\zeta(3)}\left(\frac{T}{T_{\mathrm{BEC}}}\right)^3\theta(T_{\mathrm{BEC}} - T). \tag{4.19}
$$

5 Conclusion

As we have said, in the standard theoretical treatment of the BEC problem the trap is a three-dimensional box with, importantly, a fixed volume. In this case the Bose condensate

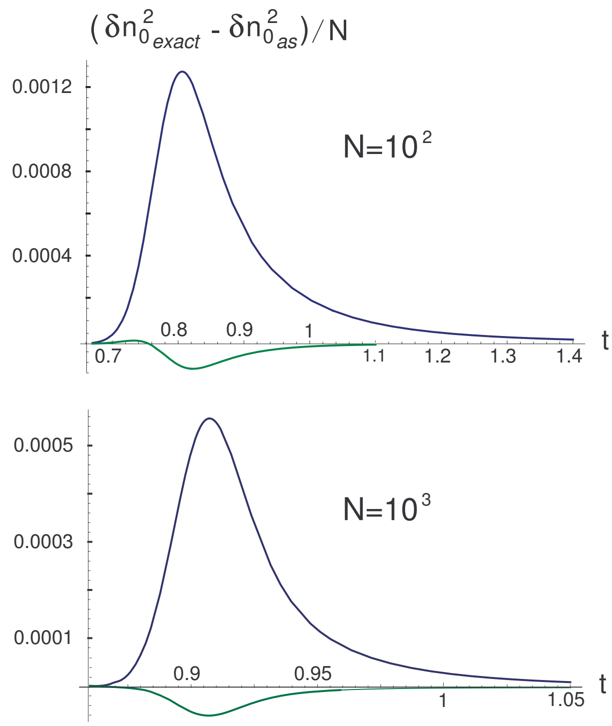

Рис. 4: The difference between the approximate expressions for the fluctuations and the exact values $(\delta \mathrm{n}_{0\,exact}^2 - \delta \mathrm{n}_{0\,as}^2)/N$. Curve 1 corresponds [see Eq. (4.15)] to the leading asymptotic contribution $f(0)$, curve 2 includes the asymptotic correction $f''(0)$.

formation temperature (on the quantum scale $\tau = T/\hbar\omega_{\rm box}$) has the form

$$\tau_{\rm BEC}^{\rm box} = \left(\frac{N}{\zeta(3/2)}\right)^{2/3}, \tag{5.1}$$

while in the problem considered above, for a trap in which the confining potential is quadratic and the volume is not fixed,

$$\tau_{\rm BEC}^{\rm trap} = \left(\frac{N}{\zeta(3)}\right)^{1/3}. \tag{5.2}$$

As is seen from Eqs. (5.1) and (5.2), the dependence of the BEC temperature on the number of particles in the system is significantly different in these two cases. For the box the characteristic energy is expressed in terms of the volume V of the system and the mass M of the particle in the following way:

$$\hbar\omega_{\rm box} = \frac{\pi^2\hbar^2}{2\,\mathrm{V}^{2/3}M}. \tag{5.3}$$

In the magnetic trap the volume is not fixed and, moreover, it changes with changing temperature. We define the effective size of the system in a trap with a quadratic confining potential as the amplitude of the oscillations of an oscillator with energy equal to the temperature T. Then

$$\mathrm{V}^{eff} \simeq \frac{4\pi}{3}\left(\frac{T}{M\omega^2}\right)^{3/2}. \tag{5.4}$$

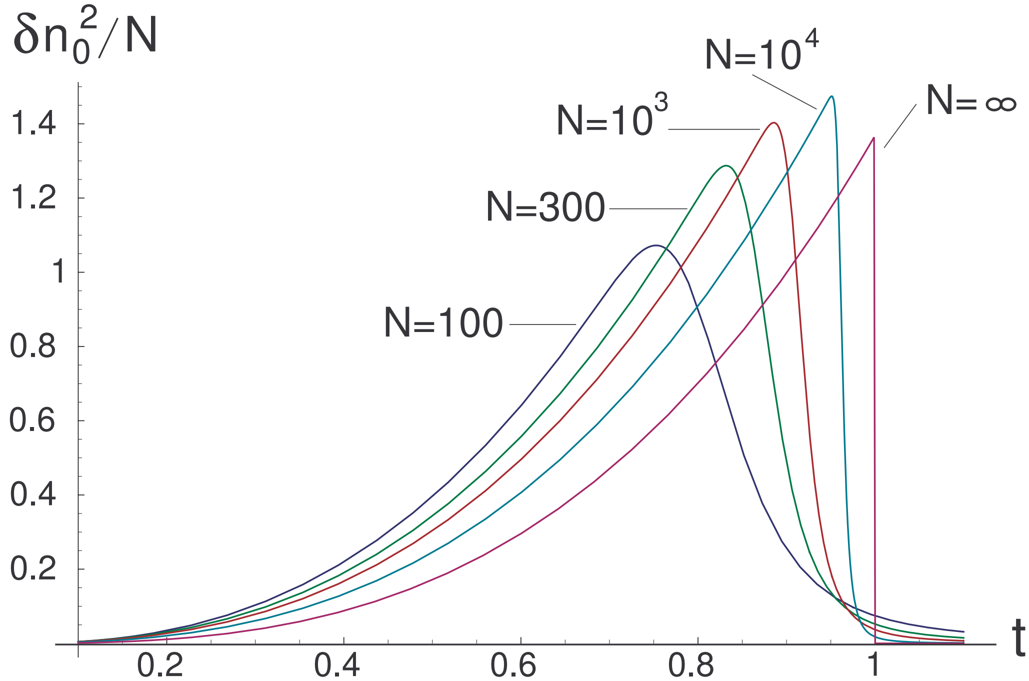

Рис. 5: Dependence of the relative fluctuation $\delta n_0/N$ on temperature $t = T/T_{BEC}$ for different values of the number of particles in the system.

Now, after expressing the number of particles in terms of the particle density ρ ($N = \rho\mathrm{V}$) and substituting Eq. (5.3) into (5.1) and (5.4) into (5.2), we find for T_{BEC} in the two cases

$$\begin{aligned} T_{\mathrm{BEC}}^{\mathrm{box}} &= \frac{\pi^2\hbar^2}{2M}\left(\frac{\rho}{\zeta(3/2)}\right)^{2/3}, \\ T_{\mathrm{BEC}}^{\mathrm{trap}} &= \frac{\hbar^2}{M}\left(\frac{4\pi\rho}{3\zeta(3)}\right)^{2/3}. \end{aligned} \tag{5.5}$$

It follows from (5.5) that in the language of particle number density the the temperatures of BEC in the box and trap are close not only qualitatively but also quantitatively:

$$\frac{T_{\mathrm{BEC}}^{\mathrm{box}}}{T_{\mathrm{BEC}}^{\mathrm{trap}}} = \frac{1}{2}\left[\frac{3\pi^2\zeta(3)}{4\zeta(3/2)}\right]^{2/3} \simeq 1.13. \tag{5.6}$$

On the whole, it should be emphasized one again that BEC is rightfully considered to be one of the fundamental discoveries of theoretical physics. Its clearest trait is not simply the accumulation of a macroscopic number of particles in the ground state upon cooling of an ideal Bose gas but the fact that this process is a phase transformation in a system of mutually *noninteracting* particles. Most likely the term "Bose condensation" came into use because of the analogy (which, strictly speaking, is not entirely correct) with the condensation of a vapor to a liquid, which was discussed by Einstein in his pioneering paper [3].

Although phase transformations in nature are extremely diverse, at the same time they demonstrate surprising universality: the change of the thermodynamic properties of a system occurs abruptly when the temperature (or some other controllable parameter) crosses its critical value. From a formal theoretical physics point of view the main question is, how, in functions which are initially analytic in temperature, does the singularity arise at the critical point T_c:

$$f(T,N) \underset{N\to\infty}{=} f_1(T)\,\theta(T_c - T) + f_2(T)\,\theta(T_c - T). \tag{5.7}$$

Bose-Einstein condensation, as an exactly solvable model, gives a simple answer to this question. For example, in the GCE the role of the "smeared" θ-function, according to Eq. (1.13), is played by the quantity

$$\theta_{\mathrm{GCA}}(x) = \frac{1}{2}\left(\frac{x}{\sqrt{x^2 + \alpha_{\mathrm{GCA}}/N}} + 1\right), \qquad \alpha_{\mathrm{GCA}} = \frac{4\zeta(2)}{\zeta(3)}, \tag{5.8}$$

and in the CE, as follows from Eq. (4.11), by

$$\theta_{\mathrm{CA}}(x) = \frac{1}{2}\mathrm{Erfc}\,(-\alpha_{\mathrm{CA}}\sqrt{N}\,x), \qquad \alpha_{\mathrm{CA}} = \sqrt{\frac{\zeta(3)}{2\zeta(2)}}. \tag{5.9}$$

For both representations (5.8) and (5.9) at $N \to \infty$ the limit is the ordinary θ-function, but at a finite value of N they behave differently. It is seen in Fig. 6 that θ_{CA} is closer to a step than θ_{GCA}. Thus one can say that the thermodynamic limit sets in somewhat faster in the CE than in the GCE.

If as the function $f(T,N)$ in (5.7) we take the specific free energy

$$f(T,N) = -\frac{T}{N}\ln Z,$$

then both $f_1(T)$ and $f_2(T)$ are identical in the two ensembles, thus implying the equivalence of the ensembles:

$$f_1(T) = -\frac{\zeta(4)}{\zeta(3)}\frac{T^4}{T^3_{\mathrm{BEC}}}, \qquad f_2(T) = -\frac{\mathrm{Li}_4(\mathrm{e}^{\mu/T})}{\zeta(3)}\frac{T^4}{T^3_{\mathrm{BEC}}}. \tag{5.10}$$

The chemical potential μ in Eq. (5.10) as a function of temperature and particle number density is the solution of the equation

$$T^3\mathrm{Li}_3(\mathrm{e}^{\mu/T}) = \zeta(3)\,T^3_{\mathrm{BEC}},$$

where $\mathrm{Li}_k(z)$ is the polylogarithm [see Appendix, Eq. (A.12)]. However, the specific fluctuations of the Bose condensate is different in the different ensembles: in the GCE

$$\lim_{N\to\infty}\frac{\delta\mathrm{n}_0^2}{N} = \begin{cases} \infty & \text{при } T < T_c, \\ 0 & \text{при } T > T_c, \end{cases}$$

and in the CE

$$\lim_{N\to\infty}\frac{\delta\mathrm{n}_0^2}{N} = \frac{\zeta(2)}{\zeta(3)}\frac{T^3}{T^3_{\mathrm{BEC}}}\,\theta(T_c - T).$$

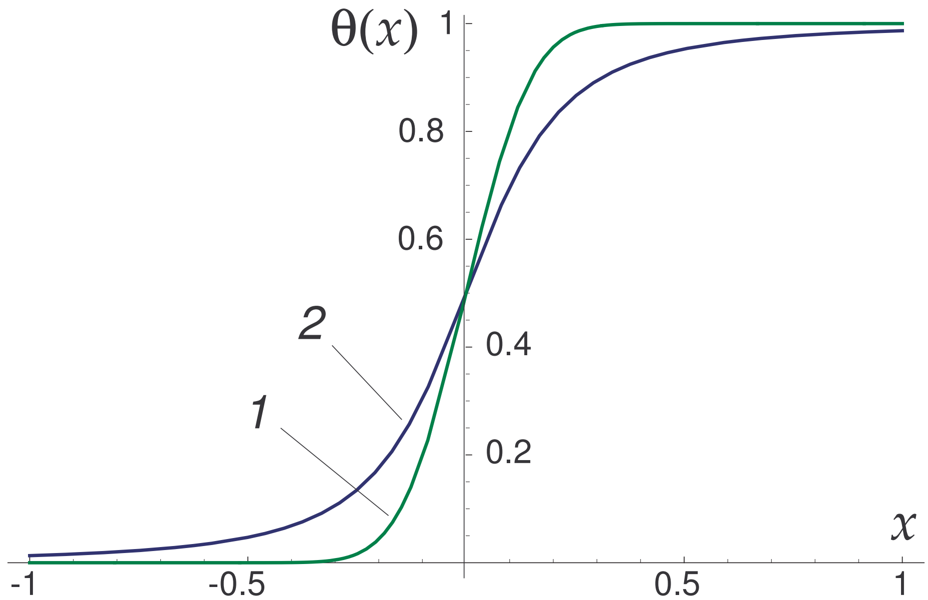

Рис. 6: Behavior of the smoothed θ-functions for $N = 10^2$. Curve 1 — $\theta_{\mathrm{CA}}(x)$, curve 2 — $\theta_{\mathrm{GCA}}(x)$.

In and of itself the accumulation of particles at the lowest energy level is the direct and rather trivial consequence of Bose statistics, evident from the form of the formulas for the average occupation numbers, Eq. (1.5). When one is talking about a phase transition, however, the question of thermodynamic limit must also be addressed: for example, is a number of particles $N = 10^3$ sufficient to approach it? To speak more precisely, the term thermodynamic limit is commonly understood to mean letting the volume of the system go to infinity at fixed temperature with the various densities (e.g., the particle number density ρ) held constant. However, the volume, density, and temperature are dimensional quantities: 1 meter is almost "infinite"if one is measuring in angstroms. >From the point of view of theoretical physics, any limit should be formulated in the language of dimensionless quantities, and in the problem of BEC of an ideal gas there are only two such quantities: the total number of particles in the system, N, and the temperature on the quantum scale, $\tau = T/\hbar\omega$. Therefore the thermodynamic limit is, first and foremost, $N \to \infty$, and the densities should be taken as the ratios of the corresponding extensive quantities to the total number of particles. The asymptotic corrections to the limit $N \to \infty$ in the our problem are of the order of $N^{-1/3}$, so that, it would seem, the thermodynamic limit is reached with 10% accuracy if $N = 10^3$. On the other hand, however, the BEC temperature for this number of particles is comparable to the ground state energy ε_0 (we recall that in the given problem $T_c \simeq 6\varepsilon_0$ at $N = 10^3$), and so one cannot speak of a macroscopic scale of the physical quantities.

In this regard we note that when atoms of alkali metals are held in magnetic traps the procedure of preparing a coherent state of N particles is said to involve “cooling” apparently to reflect its thermodynamic nature. Meanwhile, neither the volume nor the temperature nor, moreover, the spectral density of the particle number cannot be controlled

to the required precision because of technical shortcomings and for fundamental reasons: what is the temperature on quantum scales $T \sim \varepsilon_0$? Therefore, in light of the results presented above, there is ample justification for concluding that the assertion that true BEC has been observed in these undeniably outstanding experiments should be taken with a degree of caution.

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Appendix

The function $W(\nu)$ (2.10) and its derivatives $W^{(p)}(\nu)$ is determined by series of the form $\sum\limits_{l=0}^{\infty} h(l)$. Separating m the first m terms, we denote the remainder of the series as

$$K = \sum_{l=m+1}^{\infty} h(l) \tag{A.1}$$

and take an Abel-Plana transform of it. Then the series in Eq. (A.1) is transformed to the sum of two integrals,

$$K = I + J, \tag{A.2}$$

in which

$$I = \int_{m+\frac{1}{2}}^{\infty} dl\, h(l)\,, \tag{A.3}$$

$$J = -2\int_{0}^{\infty} \frac{dx\, \mathrm{Im}[h(m+\frac{1}{2}-ix)]}{\mathrm{e}^{2\pi x}+1}\,. \tag{A.4}$$

In order for series (A.1) to converge, the function $h(l)$ must fall off with increasing l not slower than l^{-1}. For a power-law function $h(l) \sim l^{-\alpha}$ its derivatives $h^{(p)}(l)$ behaves at large l as $l^{-\alpha-p}$. In this case the integral J can be evaluated with the aid of an asymptotic expansion in inverse powers of m. We expand the function $h(m+\frac{1}{2}-ix)$ in the integrand of (A.4) in a Taylor series at the point $x=0$. For the sum of any finite number n of terms in this expansion one can switch order of the summation and integration and get

$$J \simeq \sum_{l=0}^{n} (-1)^l c_l h^{(2l+1)}(m+\tfrac{1}{2}), \tag{A.5}$$

where

$$c_l = \frac{1}{(2l+1)!}\int_{0}^{\infty} \frac{dx\, x^{2l+1}}{\mathrm{e}^{2x}+1} = \frac{(1-2^{-2l-1})\zeta[2l+2]}{(2\pi)^{2(l+1)}}\,. \tag{A.6}$$

We note that the optimal number of terms in the asymptotic expansion (A.5) is determined by the form of the coefficients c_l. Therefore evaluation of the integral J can be done with the aid of (A.5) to any desired accuracy by increasing m.

We now use this technique to evaluate the logarithm of the partition function (2.2). Here the function $h(l)$ has the form

$$h(l) = g(l)\ln(n_l + 1), \tag{A.7}$$

$$g(l) = \frac{1}{2}(l+1)(l+2), \quad n_l = \frac{1}{\mathrm{e}^{(l-\sigma)/\tau} - 1}, \quad \tau = \frac{T}{\hbar\omega}, \quad \sigma = \nu\tau - \frac{3}{2}. \tag{A.8}$$

Then

$$W(\nu) = \sum_{l=0}^{m} g(l)\ln(n_l+1) + I + J. \tag{A.9}$$

The integral I in (A.9) is expressed in terms of the polylogarithms (Lerch functions)

$$I = \tau^3 \mathrm{Li}_4(z) + a\tau^2 \mathrm{Li}_3(z) + b\tau \mathrm{Li}_2(z), \tag{A.10}$$

where

$$a = g'(m+\tfrac{1}{2}) = m+2, \quad b = g(m+\tfrac{1}{2}) = \tfrac{1}{2}(m+\tfrac{3}{2})(m+\tfrac{5}{2}),$$
$$z = \mathrm{e}^{-(m+\frac{1}{2}-\sigma)/\tau}, \tag{A.11}$$

$$\mathrm{Li}_k(z) = \frac{1}{\Gamma(k)}\int_0^\infty \frac{dx\, x^{k-1}}{\mathrm{e}^x/z + 1} = \sum_{l=1}^{\infty}\frac{z^l}{l^k}, \quad \mathrm{Li}_{k-1}(z) = z\frac{d\,\mathrm{Li}_k(z)}{dz}. \tag{A.12}$$

The contribution J in (A.9) has the form

$$J = \sum_{l=0}^{n}(-1)^l c_l f_l, \tag{A.13}$$

where

$$f_0 = a\ln(r+1) - b\tau^{-1}r, \tag{A.14}$$

for $l > 0$

$$f_l = -l(2l+1)\tau^{-2l+1}r_{2l-1} + a(2l+1)\tau^{-2l}r_{2l} - b\tau^{-2l-1}r_{2l+1}, \tag{A.15}$$

$$r_0 = r = n_{m+\frac{1}{2}} = \frac{1}{\mathrm{e}^{(m+\frac{1}{2}-\sigma)/\tau} - 1}, \quad r_l = \tau^l \frac{\partial^l r}{\partial \sigma^l} = r(r+1)\frac{\partial r_{l-1}}{\partial r}.$$

For calculating the asymptotic expansion of $W(\nu)$ at large τ it is sufficient to keep only one term in the sum on the right-hand side of (A.9): ($m = 0$ in (A.1)). Then, using the well-known asymptotic expansion of the polylogarithm for $x \to 0$

$$\mathrm{Li}_4(\mathrm{e}^{-x}) = \zeta(4) - \zeta(3)x + \zeta(2)\frac{x^2}{2} + \left(\ln x - \frac{11}{6}\right)\frac{x^3}{6} + O(x^4), \tag{A.16}$$

where $\zeta(j)$ is the Riemann ζ-function

$$\zeta(4) = \frac{\pi^4}{90}, \quad \zeta(3) \simeq 1.202, \quad \zeta(2) = \frac{\pi^2}{6},$$

with accuracy up to terms that do not fall off with increasing τ we find that

$$\begin{aligned}
I = &\tfrac{\pi^4}{90}\tau^3 + g'(\sigma)\zeta(3)\tau^2 + g(\sigma)\tfrac{\pi^2}{6}\tau + \\
&+\tfrac{1/2-\sigma}{6}\left\{\left[g(\sigma+1)+\tfrac{5}{2}\right]\ln\left[\tfrac{1/2-\sigma}{\tau}\right] - \tfrac{1}{6}\left[11(\sigma+2)^2 - \sigma - \tfrac{3}{4}\right]\right\} + O(\tau^{-1}).
\end{aligned} \tag{A.17}$$

Here the contribution (A.4) takes the form

$$\begin{aligned}
J = 2\int_0^\infty \frac{dx}{\mathrm{e}^{2\pi x}+1}\mathrm{Im}\left[g(\tfrac{1}{2}-ix)\ln(1-\mathrm{e}^{-(\frac{1}{2}-\sigma-ix)/\tau})\right] \simeq \\
\simeq \frac{\ln\tau}{12} + 2\int_0^\infty \frac{dx}{\mathrm{e}^{2\pi x}+1}\mathrm{Im}\left[g(\tfrac{1}{2}-ix)\ln(\tfrac{1}{2}-\sigma-ix)\right] + O(\tau^{-1}).
\end{aligned} \tag{A.18}$$

The asymptotic expansion for the derivatives $W^{(p)}(\nu)$ we obtain by differentiating expressions (A.10) and (A.18) with respect σ:

$$W^{(p)}(\nu) = \frac{\tau^p\partial^p}{\partial\sigma^p}\left[\ln(n_0+1) + I + J\right].$$

We note that, starting with the third derivative, expression (A.10) for I can be written in terms of elementary functions, since

$$\mathrm{Li}_1(\mathrm{e}^{-x}) = -\ln(1-\mathrm{e}^{-x}). \tag{A.19}$$

The derivative $\partial J/\partial\sigma$ is expressed in terms of the special function $\psi(z) = \Gamma'(z)/\Gamma(z)$:

$$\frac{\partial J}{\partial\sigma} = -2\int_0^\infty \frac{dv}{\mathrm{e}^{2\pi x}+1}\mathrm{Im}\left[\frac{g(\frac{1}{2}-ix)}{\frac{1}{2}-\sigma-ix}\right] = \frac{1}{48} - g(\sigma)\left[\psi(1-\sigma) - \ln(\tfrac{1}{2}-\sigma)\right]. \tag{A.20}$$

In particular, for the derivative $W'(\nu) = \sum\limits_{l=0}^{\infty} g(l)n_l$ with Eq. (A.20) taken into account, we arrive at the expression

$$\begin{aligned}
W'(\nu) \;=\; & n_0 + \zeta(3)\tau^3 + g'(\sigma)\frac{\pi^2}{6}\tau^2 + \tau g(\sigma)\left[\ln\tau - \psi(1-\sigma)\right] + \\
&+\frac{\tau}{4}\left(3\sigma^2 + 5\sigma - \tfrac{19}{6}\right) + \frac{1}{6}\left(\tfrac{1}{2}-\sigma\right)\left[g(\sigma+1)+\tfrac{5}{4}\right] - \frac{1}{24} + O(\tau^{-1}).
\end{aligned} \tag{A.21}$$

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